האוניברסיטה העברית - הפקולטה לחקלאות
המכון לביוכימיה, מדעי המזון והתזונה

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הנושא:

Mapping Protein and Ligand-Protein Dynamics with Monte Carlo Techniques

המפגש יתקיים
ביום ד', 19 פברואר 2014, בשעה 10:00
מועדון סגל

Abstract:

Understanding the protein-ligand interaction mechanism requires the description of ligand migration and binding site induced fit. Such study involves dynamic time scales on the range of micro- to mili- seconds, a non-trivial task for current computational methods. Despite these difficulties, it has centered a great deal of effort from the molecular dynamics community, with its highest point, probably, in the recent design and development of the ANTON machine.[1]

Here we will present an alternative to MD techniques. Using technological advances in protein structure prediction, we have recently introduced PELE (protein energy landscape explorations). PELE combines a Monte Carlo stochastic approach with protein structure prediction algorithms and is capable of accurately reproducing long time scale processes in only few hours of CPU (typically no more than an overnight computing period).[2,3] For example, we can map de free (non biased) ligand diffusion and binding, such as the one performed with ANTON at a fraction of the cost, ~16 processors for 24 hours.[4,5] Recently, by combining PELE with markov state models (MSM), we obtained absolute binding free energies at an affordable computational cost.[6] This talk will summarize the technique, our latest studies of protein and protein-ligand dynamics, and the web server where the software is available for remote run.

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(4) Lucas, M. F.; Guallar, V. *Biochimica et biophysica acta* **2013**.
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